

4,4'-propane-1,3-diylidiphenol
2549-50-0 | DTXSID70292910

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.65e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.65e-01

Confidence level: 4.63e-01

Nearest Neighbors from the Training Set

Image not found

1,3-Naphthalenediol

Measured: 1.12e-02

Predicted: 2.01e-02

Image not found

1,5-Dihydroxynaphthalene

Measured: 1.03e-03

Predicted: 8.87e-03

Image not found

3-Amino-3-(naphthalen-1-yl)propanoic acid

Measured: 2.57e-02

Predicted: 1.36e-02

Image not found

2,3-Dihydroxynaphthalene

Measured: 1.83e-03

Predicted: 3.03e-02